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14. ABSTRACT
This work explores possible cross-slip mechanisms of gliding type <*a*> = *a*/3[1 -2 1 0] dislocation loops in wurtzite gallium nitride (GaN) as a function of slip plane. A modified form of the dislocation dynamics code Para-DiS was employed using isotropic linear elasticity and dislocation mobilities estimated in part from molecular dynamics (MD) simulations. Under an externally applied uniform stress, the occurrence of cross slip events is highly dependent on the initial dislocation slip plane. The basal plane is the preferred active plane, owing to the greater mobility of <*a*> type segments on that plane, over the other planes considered including the prismatic (-1 0 1 0) and two equivalent pyramidal planes (-1 0 1 1) and (1 0 -1 1). For an applied stress state, cross-slip processes are more readily seen from the prismatic-to-basal planes or the pyramidal-to-basal planes, and neither is found to occur in reverse. Cross slip by climb is not presently considered. In all cases, cross-slip events occur after the loop expands until a greater number of screw-oriented segments are able to access the cross-slip plane and the resolved stresses on the plane become sufficiently large. In comparison with dislocations found in GaN previously, the calculations suggest that some threading dislocations along the [0001] direction that have edge character may have been formed from loops whose screw segments slip and escape on basal planes leaving only the edge segments.

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Cross slip of dislocation loops in GaN under shear

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This work explores possible cross-slip mechanisms of gliding type <*a*> = *a*/3[1 -2 1 0] dislocation loops in wurtzite gallium nitride (GaN) as a function of slip plane. A modified form of the dislocation dynamics code ParaDiS was employed using isotropic linear elasticity and dislocation mobilities estimated in part from molecular dynamics (MD) simulations. Under an externally applied uniform stress, the occurrence of cross slip events is highly dependent on the initial dislocation slip plane. The basal plane is the preferred active plane, owing to the greater mobility of <*a*> type segments on that plane, over the other planes considered including the prismatic (-1 0 1 0) and two equivalent pyramidal planes (-1 0 1 1) and (1 0 -1 1). For an applied stress state, cross slip processes are more readily seen from the prismatic-to-basal planes or the pyramidal-to-basal planes, and neither is found to occur in reverse. Cross slip by climb is not presently considered. In all cases, cross-slip events occur after the loop expands until a greater number of screw-oriented segments are able to access the cross slip plane and the resolved stresses on the plane become sufficiently large. In comparison to dislocations found in GaN previously, the calculations suggest that some threading dislocations along the [0001] direction that have edge character may have been formed from loops whose screw segments slip and escape on basal planes leaving only the edge segments.

1 Introduction In recent years, (Al)GaN wurtzite semiconductors have attracted much attention due to their many unique features as possible replacements of Si-based and conventional III-V structures such as $Al_xGa_{1-x}As$ [1-5]. However, severe performance degradation due to dislocations in the structure has severely inhibited the realization of many potential applications [6-9]. Even though heteroepitaxial wurtzite structures can now be successfully fabricated on GaN substrates with relatively small dislocation densities below 10^6 cm^{-2} [10, 11], detailed mechanisms that explain how and why threading configurations form still remain elusive. Unlike zinc blende semiconductors such as $Si_{1-x}Ge_x$ for which the dislocation mechanisms have been widely studied [12, 13], this body of knowledge applicable to dislocations in cubic crystals does not easily apply to hexagonal crystals such as the (Al)GaN family. In particular, information on cross slip mechanisms for dislocations in (Al)GaN is scarce though possible cross slip mechanisms have been suggested by cathodoluminescence (CL) images of dislocations in GaN under indentation [14]. These have shown that slip processes are sensitive to the complexity of multiple available slip systems unique to hexagonal close-packed (*hcp*) and wurtzite crystals. Therefore, it is important to understand cross slip of dislocations in GaN to find possible mechanisms that explain how and why dislocations form on certain planes during growth. This work explores dislocation evolution due to cross slip and examines the inter-correlations between simulated dislocation configurations to those reported experimentally.

2 Simulations and methodology

2.1 Discrete dislocation dynamic (DDD) simulations In this work, we employ a modified version of the ParaDiS code [15, 16]. First a simulation box of dimension

600,000a is created. Then a circular dislocation loop of 5 micron radius is placed at the center of the box either on the basal, prismatic, or pyramidal plane. The loop is allowed to evolve under an externally applied stress with an overall magnitude of ~0.1 GPa. The applied stress tensor is given in its symmetric form as (σ_{xx},σ_{yy},σ_{zz},σ_{xy},σ_{zx},σ_{yz}) = (-0.41, -0.63, 0.00, -0.21, -0.05, -0.20) GPa. Here the orthogonal coordinates are defined such that the z-axis is along the c-axis while the x and y axes are along and bisecting a prismatic plane, namely, along the [1 1 -2 0] and [1 -1 0 0] directions, respectively. The values are derived to match the critical resolved shear stress needed to observe dislocation glide in wurtzite nitride semiconductors to ensure the resolved shear stresses are of sufficient magnitude for the dislocation loops to glide and experience cross slip onto alternate planes, cf. [14, 17, 18]. The stress components are reminiscent of state at a location offset from the loading axis beneath a point tip. They are obtained by superposition of each projection stress tensor determined by the plane normal and the Burgers vector [19]. We have also performed simulations of $Al_{0.49}Ga_{0.51}N$ using identical slip systems and initial configurations for the dislocation loop in order to compare the simulated dislocation configurations with dislocation images reported previously [20]. The isotropic elastic constants used in this work are specified in Table 1 [21]. The values for $Al_{0.49}Ga_{0.51}N$ are derived from those of bulk GaN and AlN by interpolating linearly to the composition of 51% for Ga.

Table 1 The isotropic elastic constants used in this work.

Material	a (Å)[$]	c/a[&]	μ (GPa)	ν
GaN	3.19	1.6277	207	0.202
$Al_{0.49}Ga_{0.51}N$	3.15	1.6141	208	0.206

[$,&] a and c refer to the lattice spacings in the basal plane and its normal directions, respectively.

The ParaDiS implementation of cross slip is briefly described for the sake of readability. For cross slip to occur in the present simulations, two conditions must be met. First, the dislocation segments must be of predominantly screw character and, secondly, the critical resolved shear stress must be larger on the secondary plane for the dislocation to undergo a cross slip process away from the original primary plane. In terms of the implementation, when any node is connected to a segment that is within a small tolerance of being screw-type, and the critical resolved shear stress on the secondary plane is larger than a small value greater than the stress on the primary plane, the segment will cross slip.

2.2 Molecular dynamics simulations Previously [22], classical MD simulations were performed using the LAMMPS computer code [23] to calculate the average velocity of edge dislocations as a function of applied stress gliding on basal, prismatic, and pyramidal planes with an active Burgers vector of type <a> at 1300 K. The mobilities in the present paper are defined using a linear combination of the perfect edge mobilities from the results of [22] and estimated values of screw mobilities [24]. The earlier MD simulations of edge dislocations tested a large range of stresses which yielded nonlinear behavior in the mobility [22]. Thus, the present values are obtained from a linear fit to only a portion of the earlier simulated stress range. These values are listed in Table 2. The screw mobilities shown are estimated using observed ratios between edge and screw dislocations on different planes for *hcp* metals [24].

Table 2 The drag coefficients as functions of slip plane for screw (B_s) and edge (B_e) dislocations.

Slip plane	B_s (Pa s)	B_e (Pa s)
basal	0.107	0.036
prismatic	0.290	0.058
pyramidal	107.400	107.400

Noteworthy is that the drag coefficients in Table 2 for the basal plane is three orders of magnitude smaller than the pyramidal plane and approximately 60% smaller than the prismatic plane. The mobility values are qualitatively consistent with earlier reports of dislocation motion in *hcp*-based structures. Staroselsky and Anand's constitutive model for Mg alloys proposed a three orders of magnitude larger resistance for the slip on the prismatic and pyramidal planes than on the basal plane [25]. For dislocations in GaN [26], it was suggested that dislocations on (0 0 0 1) basal planes appeared to be more mobile than those on {1 -1 0 0} prismatic planes due to the shorter distance between the Peierls valleys and the greater distance between the parallel planes for the basal than the prismatic planes.

3 Results and discussions Using type <a> Burgers vector and the uniform stress state, the simulation results indicate that when cross slip occurs, basal planes are the preferred planes on to which accessible segments will cross slip and glide. This holds true independent of the primary plane of the loop and regardless of whether the material is GaN or $Al_{0.49}Ga_{0.51}N$. A loop that starts on the basal plane is not observed cross slipping on to the prismatic or pyramidal plane whereas those initially on the prismatic or pyramidal plane appear to cross slip readily to parallel basal planes, as shown in Figs. 1 and 2. The portion of the dislocation loop that remains on the prismatic or pyramidal plane has strong edge character. The dislocation segments interact with each other [27] and, through balance from line tension effects, gradually evolve into parallel edge dislocation dipoles. The location at which the portions of the former single-plane loop intersects the new plane becomes a constriction point on the basal plane and a source for further generation of Frank-Read loops [28]. However, owing to the fact that these are now on the basal plane, they do not possess any threading component nor cross slip onto other planes.

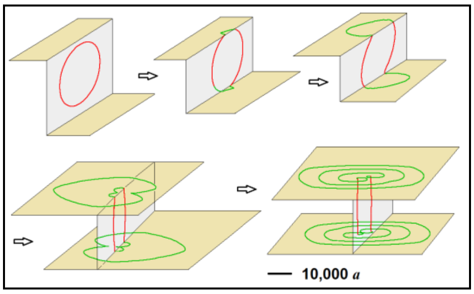

Figure 1 Evolution of a dislocation loop initially on the (-1 0 1 0) prismatic plane cross slips to the basal planes. Green dislocations are on the basal planes (the yellow shaded areas) and those in red are on the prismatic plane (the grey shaded area).

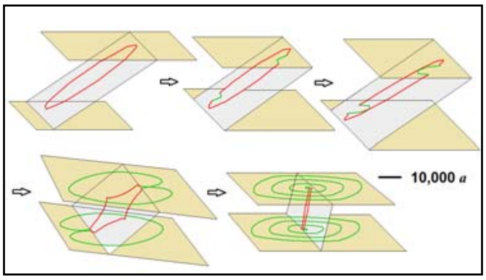

Figure 2 Evolution of a dislocation loop initially on the (-1 0 1 1) pyramidal plane cross slips to the basal planes. Green dislocations are on the basal planes (the yellow shaded areas) and those in red are on the pyramidal plane (the grey shaded area).

The configurations of our simulated dislocation configurations, especially the nearly-parallel dislocation lines along the vertical and pyramidal directions strongly resembles the threading dislocations previously reported in (Al)GaN [20, 26]. In Sugiura's study [26], wind-shaped dislocations were observed on the basal (0001) plane as extensions from the vertical edge threading dislocations on {1 -1 0 0} prismatic planes with the type <*a*> active Burgers vectors. In Cantu et al's study [20] on the threading dislocations in $Al_{0.49}Ga_{0.51}N$ strained layers, it is reported that dislocations gliding on the prismatic plane were inclined ~15^o to 25^o from the *c*-axis on possible {1 -1 0 0} prismatic planes.

The loops in $Al_{0.49}Ga_{0.51}N$ also show the same range of inclination angles between the segments on the primary and secondary slip planes. As shown in Fig. 3, the inclination angle of the first threading segment is computed to be approximately 20^o. The inclination is a consequence of the competition between the segment interactions, the externally applied force, and the self force.

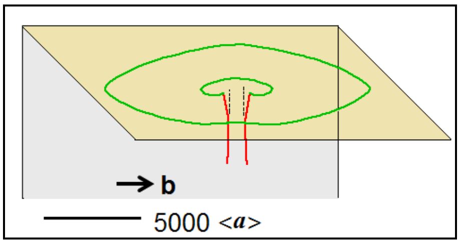

Figure 3 Simulated dislocation inclination on the prismatic plane from the *c*-axis. Evolution of a dislocation loop initially on the (-1 0 1 1) pyramidal plane cross slips to the (0 0 0 1) basal plane. The dislocation portions shown in green are on the basal plane (the yellow shaded area) and those in red are on the prismatic plane (the grey shaded area).

Figure 4 depicts the changes in character of a portion of the dislocation loop that undergoes cross-slip from the prismatic plane to the basal plane. As the loop expands prior to cross slip in Fig. 4(a), more dislocation segments take on screw character. The simulation indicates the segments between nodes #2 and #12 in Fig. 4(b) at the 550 timestep are nearly screw. After the cross slip process occurs where node #21 already crosses from the primary prismatic plane to the secondary basal plane, the loop on the basal plane continues to bow out and become more edge-like under the influence of the applied stress, as shown in Fig. 4 (c).

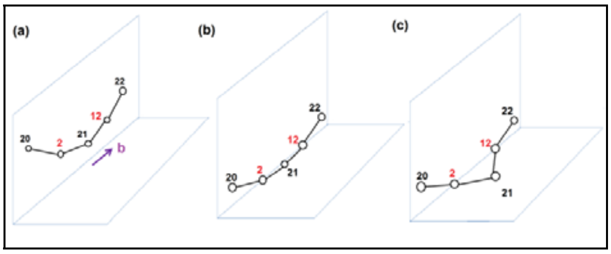

Figure 4 A schematic depicting the changes in characters for the dislocation segments prior to and after cross-slip from the prismatic plane to the basal plane at timestep = (a) 300, (b) 550, and (c) 700. The numbers are the node tags in the simulation.

The changes in nodal forces during the cross slip process have also been studied. Using the #2, #12 and #21 nodes in Fig. 4, the magnitudes of the forces projected along the basal, prismatic, and pyramidal planes are evaluated with respect to simulation time and are shown in Fig. 5.

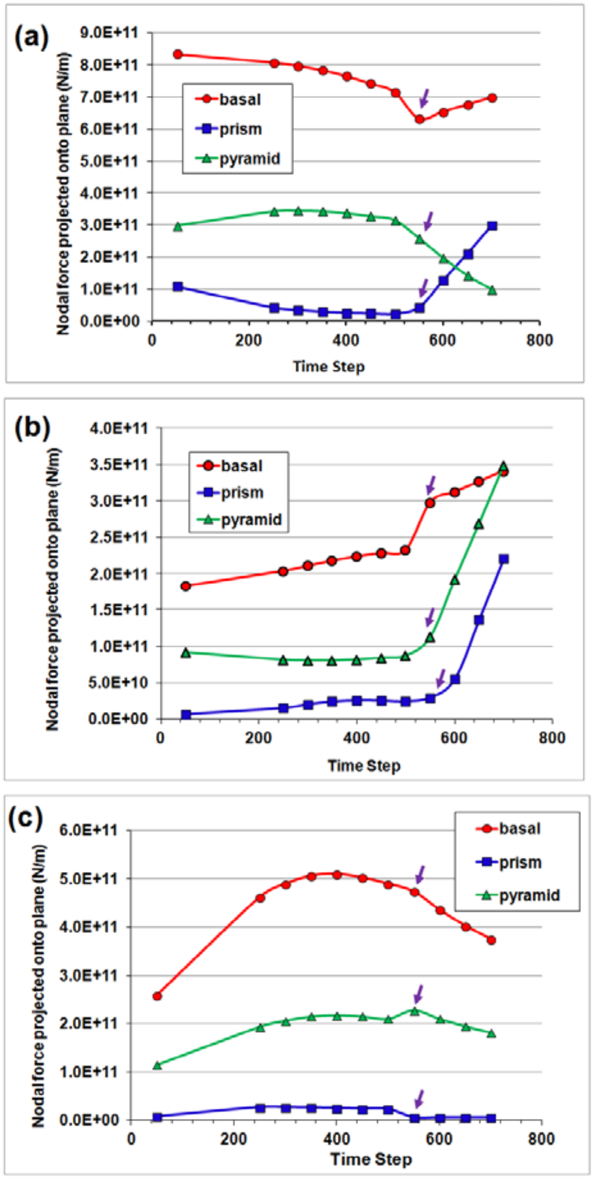

Figure 5 The corresponding forces acting on the nodes, (a) node #2, (b) node #12, and (c) node #21, as depicted in Fig. 4, projected on to different possible slip planes. The small arrows indicate the occurrence of cross slip.

Initially, node #2 has driving forces on the basal plane that may be eight times and twice larger than those on the prismatic and pyramidal planes, respectively. For node #12, the driving forces on the basal plane are one-order of magnitude larger than those on the other planes. This corresponds to a period when the loop grows exclusively on the primary prismatic plane and the segment configurations are changing such that, with a larger radius of curvature, at least one segment is becoming more screw-like as depicted in Fig. 4. As cross slip occurs sometime between timestep 500 and 600, indicated by the small arrows in Fig. 5, the force components on the planes change drastically for nodes #2 and #12. Though Figs. 5(a) and 5(b) depict the projected forces on the two nodes #2 and #12 whose appearance is symmetric with respect to an unseen center plane that bisects the loop, the applied stress is not aligned with the local coordinate system and is also skew with respect to the local line sense of the segments attached to those nodes. Thus, it is not expected that the force vectors at the two nodes are identical.

Finally, having observed possible trends from simulations, some noteworthy inferences may be drawn about the potential connections to unexplained observations. The calculations quite clearly suggest the likelihood of cross slip as a pathway for the evolution of threading dislocations during the growth of (Al)GaN structures. The bending and tilting configurations of threading dislocations previously identified with microscopic approaches, i.e. ([14, 20, 26]) may be the results of Shockley glide loops that were initially nucleated on a primary slip plane such as the prismatic or pyramidal plane that eventually undergoes a cross slip process onto the basal plane. Furthermore, given the dependence of dislocation mobility on the slip plane as listed in Table 2 and the given stress state presently considered, it appears less probable for a dislocation to cross slip from the basal plane to either the prismatic or the pyramidal plane. The stress state favors slip on the basal plane owing to the largest component of the Peach-Koehler force in that direction. Cross slip processes tend to drive dislocation segments onto those planes and, consequently, minimize line lengths of the remaining segments of edge character in the threading direction. These observations, however, should not be confused as being conclusive about screw-type threading dislocations that are rarer than edge-type but more influential on electronic device properties nor of the likelihood of cross slip processes involving a basal primary plane.

4 Conclusions The cross slip mechanisms of different dislocation loops have been studied via DDD simulations using the type <*a*> active Burgers vector $a/3[1\ {-2}\ 1\ 0]$ and dislocation mobilities derived from MD simulations. Dislocation loops originally on prismatic or pyramidal planes tend to cross slip easily on to basal planes. The simulated dislocation configurations after cross slip resemble those of previously reported threading dislocations in (Al)GaN in terms of dislocation bending and inclination. It is possible that cross slip plays an important role in the development of threading dislocations during the growth of (Al)GaN crystals.

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